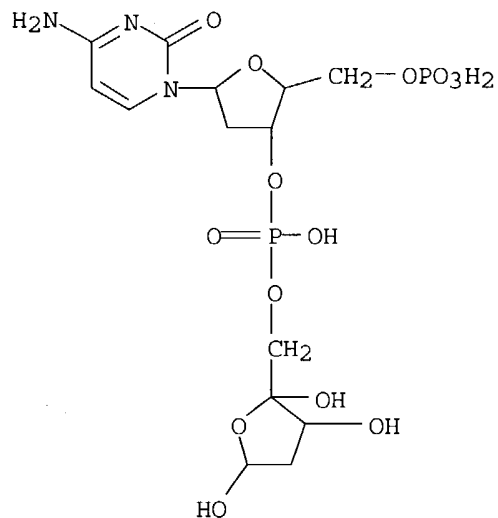


L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 127383-18-0 REGISTRY
 ED Entered STN: 01 Jun 1990
 CN 3'-Cytidylic acid, 2'-deoxy-, mono[(tetrahydro-2,3,5-trihydroxy-2-furanyl)methyl] ester, 5'-(dihydrogen phosphate) (9CI) (CA INDEX NAME)
 MF C14 H23 N3 O14 P2
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C4O	OC4	5	C4O	16.138.1	2
C4N2	NCNC3	6	C4N2	46.195.28	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	1	pH 8	(1) ACD
Bioconc. Factor (BCF)	1	pH 10	(1) ACD
Boiling Point (BP)	846.1+/-75.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (Hvap)	139.81+/-6.0 kJ/mol		(1) ACD
Flash Point (FP)	465.5+/-66.7 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	16		(1) ACD
H acceptors (HAC)	17		(1) ACD
H donors (HD)	8		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD

Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	1	pH 8	(1) ACD
Koc (KOC)	1	pH 10	(1) ACD
logD (LOGD)	-7.31	pH 1	(1) ACD
logD (LOGD)	-8.15	pH 4	(1) ACD
logD (LOGD)	-10.11	pH 7	(1) ACD
logD (LOGD)	-10.49	pH 8	(1) ACD
logD (LOGD)	-10.59	pH 10	(1) ACD
logP (LOGP)	-4.569+/-0.723		(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	519.29		(1) ACD
pKa (PKA)	1.37+/-0.50	Most Acidic	(1) ACD
pKa (PKA)	4.47+/-0.45	Most Basic	(1) ACD
Vapor Pressure (VP)	2.77E-33 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 113:20465 CA
TI Specific detection of C-4' hydroxylated abasic sites generated by bleomycin and neocarzinostatin in DNA
AU Sugiyama, Hiroshi; Kawabata, Hiroshi; Fujiwara, Tsuyoshi; Dannoue, Yukihiro; Saito, Isao
CS Fac. Eng., Kyoto Univ., Kyoto, 606, Japan
SO Journal of the American Chemical Society (1990), 112(13), 5252-7
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
CC 9-15 (Biochemical Methods)
Section cross-reference(s): 1, 6
AB This specific detection and quantitation method was based on a chemical and enzymic transformation of C-4' hydroxylated abasic sites to deoxynucleoside (3'-(3-pyridazinylmethyl) phosphates. Enzymic digestion of 3'-(3-pyridazinylmethyl) 2'-deoxycytidyl-(3'-5')-2'-deoxy-3'-guanylate with snake venom phosphodiesterase (s.v. PDE) and alkaline phosphatase (AP) gave 2'-deoxycytidine and 3'-(3-pyridazinylmethyl) 2'-deoxyguanylate (I) in high yields, indicating that a pyridazine-substituted phosphodiester bond at the 3'-end resists digestion with s.v. PDE. Enzymic digestion of d(CGCGAATTCGCG) treated with photoactivated green cobalt-peplomycin (Co·PEM) with s.v. PDE and AP following treatment with aqueous hydrazine was examined. Consistent with the previous results on the cleavage of this dodecanucleotide, I was obtained as a major product. Photoactivated Co·PEM also mediated spontaneous thymine release from poly(dA-dT) with formation of 3'-(3-pyridazinylmethyl) 2'-thymidylate (II) and 3'-(3-pyridazinylmethyl) 2'-deoxyadenylate (III). Digestion of Co·PEM-treated calf thymus DNA having a C-4' hydroxylated abasic site gave pyridazine derivs. 3'-(3-pyridazinylmethyl) 2'-deoxycytidylate (IV), 3'-(3-pyridazinylmethyl) 2'-deoxyguanylate (V), II, and III, and the total amount of II-V corresponded well to the sum of spontaneously released free bases. Also investigated was the formation of II-V in Fe·PEM- and

neocarzinostatin (NCS)-mediated degradation of calf thymus DNA. Hydrazine treatment of their reaction mixts. followed by enzymic digestion produced pyridazine derivs. II-V, indicating that C-4' hydroxylated abasic sites are actually produced in calf thymus DNA. Quant. anal. indicated that C-4' hydroxylation is estimated to be a min. of 17% of the total event caused by the action of NCS on calf thymus DNA.

- ST C 4 prime hydroxylated DNA detection; DNA hydroxylated abasic site detection; bleomycin site detection DNA; neocarzinostatin site detection DNA; deoxynucleoside pyridazinylmethylphosphate DNA; pyridazine deriv DNA abasic site; hydrazine DNA abasic site detection
- IT Deoxyribonucleic acids
RL: ANT (Analyte); ANST (Analytical study)
(abasic site-containing, 4'-hydroxy, detection of, chemical-enzymic)
- IT Nucleotides, esters
RL: PROC (Process)
(deoxyribo-, 3'-phosphates, esters, with pyridazinylmethanol, detection of, in DNA C-4'-hydroxylated abasic site detection)
- IT 127383-18-0 127383-19-1 127383-20-4 127383-21-5
RL: ANST (Analytical study)
(C-4'-hydroxylated abasic site detection in, chemical-enzymic)
- IT 26966-61-0 77889-82-8 89946-60-1
RL: ANST (Analytical study)
(C-4'-hydroxylated abasic sites detection in, chemical-enzymic)
- IT 9014-02-2, Neocarzinostatin 11056-06-7, Bleomycin
RL: ANST (Analytical study)
(DNA C-4'-hydroxylated abasic sites generated by, detection of, chemical-enzymic)
- IT 2147-15-1
RL: ANST (Analytical study)
(binding release from, detection of, chemical-enzymic)
- IT 9001-78-9, Alkaline phosphatase 9025-82-5, Phosphodiesterase 302-01-2, Hydrazine, uses and miscellaneous
RL: ANST (Analytical study)
(in DNA C-4'-hydroxylated abasic site detection)
- IT 7646-79-9DP, Cobalt chloride (CoCl₂), complexes with peplomycin sulfate 70384-29-1DP, Peplomycin sulfate, complexes with cobalt chloride
RL: PREP (Preparation)
(preparation and DNA modification by, abasic site determination in relation to)
- IT 127383-28-2P 127383-29-3P 127400-46-8P 127400-47-9P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
- IT 124842-88-2P 124842-89-3P 124863-38-3P 125198-66-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and detection of, in DNA C-4'-hydroxylated abasic site detection)
- IT 127383-22-6P 127383-23-7P 127383-24-8P 127383-25-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and enzymic digestion of)
- IT 127383-30-6P 127383-31-7P 127383-32-8P 127400-48-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with hydrazine)
- IT 78272-53-4 81187-01-1 81187-02-2 81196-20-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dimethoxydihydrofurfuryl alc.)
- IT 111026-37-0 127383-26-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phosphodiesterase and alkaline phosphatase)
- IT 19969-71-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with protected deoxyribonucleotides)